Detailed structure and transformations of grain boundaries in graphene

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Ideal graphene is formed our of an infinite array of interconnected carbon hexagons. However, large real-life graphene sheets are often not formed of a single crystal domain, but rather consist of multiple differently oriented grains connected by grain boundaries (albeit micromechanically cleaved graphene flakes are monocrystalline). With chemical vapour desposition (CVD) technique, which is perhaps the most promising route to large scale fabrication of graphene, grain boundaries are always present, although recent developments have significantly increased the typical crystal domain sizes.

Several works have been dedicated to the structure of graphene grain boundaries, as they can significantly alter the properties of graphene. However, often the detailed structure of observed grain boundaries in, e.g., high resolution transmission electron microscope (HRTEM) experiments [1] differ significantly from the theoretically proposed optimal boundaries [2].

In this work the gap between the experimental and theoretical observations is bridged by means of multiscale atomistic simulations and HRTEM experiments. A theoretical model is presented, which reproduces charasteristic features observed in real grain boundaries and predicts low energy transformation routes connecting different low-energy boundary configurations.

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[2] O. V. Yazyev and S. G. Louie Phys. Rev. B. 81 (2010) 195420